

1,3-Pentadiene, 2-methyl-

Other names:	1,3-Dimethyl-1,3-butadiene 2,4-Dimethyl-1,3-butadiene 2-Methyl-1,3-pentadiene 2-Methyl-1,3-pentadiene,c&t 2-methylpenta-1,3-diene CH2=C(CH3)CH=CHCH3
Inchi:	InChI=1S/C6H10/c1-4-5-6(2)3/h4-5H,2H2,1,3H3
InchiKey:	RCJMVGJKROQDCB-UHFFFAOYSA-N
Formula:	C6H10
SMILES:	C=C(C)C=CC
Mol. weight [g/mol]:	82.14
CAS:	1118-58-7

Physical Properties

Property code	Value	Unit	Source
affp	864.90	kJ/mol	NIST Webbook
basg	836.00	kJ/mol	NIST Webbook
gf	159.15	kJ/mol	Joback Method
hf	65.69	kJ/mol	Joback Method
hfus	8.91	kJ/mol	Joback Method
hvap	28.32	kJ/mol	Joback Method
ie	8.47 ± 0.02	eV	NIST Webbook
ie	8.42	eV	NIST Webbook
log10ws	-2.04		Crippen Method
logp	2.139		Crippen Method
mcvol	86.800	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
rinpol	624.00		NIST Webbook
rinpol	629.00		NIST Webbook
rinpol	635.00		NIST Webbook
rinpol	630.00		NIST Webbook
rinpol	624.00		NIST Webbook
rinpol	630.00		NIST Webbook
rinpol	629.00		NIST Webbook
tb	337.40	K	Joback Method
tc	517.19	K	Joback Method
tf	136.58	K	Joback Method

vc	0.334	m ³ /kmol	Joback Method
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	132.16	J/mol×K	337.40	Joback Method
cpg	142.08	J/mol×K	367.36	Joback Method
cpg	151.51	J/mol×K	397.33	Joback Method
cpg	160.47	J/mol×K	427.29	Joback Method
cpg	168.98	J/mol×K	457.26	Joback Method
cpg	177.07	J/mol×K	487.22	Joback Method
cpg	184.75	J/mol×K	517.19	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.54766e+01
Coeff. B	-3.37641e+03
Coeff. C	-3.80470e+01
Temperature range (K), min.	258.25
Temperature range (K), max.	370.20

Sources

The Yaws Handbook of Vapor Pressure: Crippen Method:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://link.springer.com/article/10.1007/BF02311772
	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1118587&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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